

Hidden Integrability of a Kondo Impurity in an Unconventional Host

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We study a spin- $\frac{1}{2}$ Kondo impurity coupled to an unconventional host in which the density of band states vanishes either precisely at (“gapless” systems) or on some interval around the Fermi level (“gapped” systems). Despite an essentially nonlinear band dispersion, the system is proven to exhibit hidden integrability and is diagonalized exactly by the Bethe ansatz.

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In the Bethe ansatz (BA) approach to the theory of dilute magnetic alloys [1,2], initiated by Wiegmann [3,4] and Andrei [5], the conditions of (i) a linear dispersion of band electrons near the Fermi level and (ii) an energy independent electron-impurity coupling play such a crucial role that up to recent time they have been considered as necessary mathematical conditions for integrability of impurity models. However, it has recently been found [6] that integrability of the degenerate and $U \rightarrow \infty$ nondegenerate Anderson models is not destroyed by a nonlinear dispersion of particles and an energy dependent hybridization, but it becomes only hidden [7]. The approach developed has allowed one to study the ground state properties of a $U \rightarrow \infty$ Anderson impurity embedded in unconventional Fermi systems, such as a BCS superconductor [8] and a “gapless” host [9]. In the latter, a density of band states is assumed to vanish precisely at the Fermi level [10].

In the BA approach, the spectrum of a metal host is alternatively described in terms of interacting charge and spin excitations rather than in terms of free particles with spin “up” and “down”. A choice of an appropriate Bethe basis of a host is dictated by physical properties of an impurity. In the Anderson model, spin and charge excitations strongly interact, while in exchange models, they are decoupled from each other. The latter stems from a momentum independence of electron-impurity scattering in exchange models. The Kondo model is thus “simpler” than the Anderson one, and its solution is derived from that of the Anderson model in the limit where an impurity energy lies much below the Fermi level of a host.

However, in an unconventional host electron-impurity scattering amplitudes even in exchange models are clear to depend essentially on an electron momentum due to an energy dependent density of band states. Therefore, charge and spin degrees of freedom in exchange models should be coupled to each other, that could lead to novel features of the Kondo physics of unconventional Fermi systems.

In this Letter, we report first results for the Kondo model in an unconventional host. Despite an essentially nonlinear dispersion of band electrons near the Fermi level, the model is proven to exhibit hidden integrability. As in the unconventional Anderson model [6], an auxiliary τ -space related to the particle energy is introduced to show that the multiparticle scattering process is factorized into two-particle ones. Multiparticle functions in an auxiliary x -space related to the particle momentum are then found as a result of an integral “dressing” procedure of the BA functions in the τ -space. Thus, factorizability of scattering in the x -space is hidden and becomes visible only in the limit of large interparticle separations.

Integrability of the unconventional Kondo model is clear to provide us a powerful theoretical tool in studies of the Kondo physics in such systems of fundamental interest as superconductors and unconventional Fermi systems, where a band particle dispersion cannot be linearized near the Fermi level.

We start with the standard s-d exchange (Kondo) model with an arbitrary band electron dispersion $\epsilon(k)$. An effective 1D Hamiltonian of the model is written in terms of the Fermi operators $c_\sigma^\dagger(\epsilon)$ [$c_\sigma(\epsilon)$] which create (annihilate) an electron with a spin $\sigma = \uparrow, \downarrow$ in an s-wave state of energy ϵ ,

$$H = \sum_{\sigma} \int_C \frac{d\epsilon}{2\pi} \epsilon c_\sigma^\dagger(\epsilon) c_\sigma(\epsilon) + \sum_{\sigma, \sigma'} \int_C \frac{d\epsilon}{2\pi} \frac{d\epsilon'}{2\pi} I(\epsilon, \epsilon') c_\sigma^\dagger(\epsilon) \left(\vec{\sigma}_{\sigma\sigma'} \cdot \vec{S} \right) c_{\sigma'}(\epsilon'). \quad (1)$$

Here, $\vec{\sigma}$ are the Pauli matrices, \vec{S} is the impurity spin operator. An effective electron-impurity coupling $I(\epsilon, \epsilon') = \frac{1}{2} I \sqrt{\rho(\epsilon)\rho(\epsilon')}$ combines the exchange coupling constant I and the density of band states $\rho(\epsilon) = dk/d\epsilon$. The integration contour C contains two intervals, $C = (-D, -\Delta) \oplus (\Delta, D)$, where D is the half band width, and 2Δ is the energy gap in a gapped host, while in a gapless host $\Delta = 0$. In what follows, we restrict our consideration to the case of $S = \frac{1}{2}$. The electron energies and momenta in Eq. (1) and hereafter are taken relative to the Fermi values, which are set to be equal to zero.

We look for one-particle eigenstates of the system in the form

$$|\Psi_1\rangle = \sum_{\sigma} \sum_{s=0,1} \int_C \frac{d\epsilon}{2\pi} \psi_{\sigma;s}(\epsilon) c_{\sigma}^{\dagger}(\epsilon) (S^+)^s |0\rangle, \quad (2)$$

where the vacuum state $|0\rangle$ contains no electrons and the impurity spin is “down”. The Schrödinger equation for the auxiliary wave function $\phi_{\sigma;s}(\epsilon) = \psi_{\sigma;s}(\epsilon)/\sqrt{\rho(\epsilon)}$ is easily found to be

$$(\epsilon - \omega)\phi_{\sigma;s}(\epsilon|\omega) + \frac{1}{2}I \left(\vec{\sigma}_{\sigma\sigma'} \cdot \vec{S}_{ss'} \right) A_{\sigma';s'}(\omega) = 0 \quad (3a)$$

$$A_{\sigma;s}(\omega) = \int_C \frac{d\epsilon}{2\pi} \rho(\epsilon) \phi_{\sigma;s}(\epsilon|\omega), \quad (3b)$$

where ω is the eigenenergy.

To simplify notation we omit hereafter the spin indexes. Inserting the general solution of Eq. (4a),

$$\phi(\epsilon|\omega) = 2\pi\delta(\epsilon - \omega)\chi - \frac{\frac{1}{2}I}{\epsilon - \omega - i0} \left(\vec{\sigma} \cdot \vec{S} \right) A(\omega), \quad (4a)$$

with an arbitrary spinor χ , into Eq. (4b), one obtains

$$\left[1 + \frac{1}{2}I\Sigma(\omega) \left(\vec{\sigma} \cdot \vec{S} \right) \right] A(\omega) = \rho(\omega)\chi. \quad (4b)$$

Here, the self-energy $\Sigma(\omega)$ is found to be

$$\Sigma(\omega) = \int_C \frac{d\epsilon}{2\pi} \frac{\rho(\epsilon)}{\epsilon - \omega - i0} = P \int_C \frac{d\epsilon}{2\pi} \frac{\rho(\epsilon)}{\epsilon - \omega} + \frac{i}{2}\rho(\omega) = \Sigma'(\omega) + i\Sigma''(\omega), \quad (5)$$

where P stands for the principal part.

It is convenient to rewrite Eq. (3a) for the Fourier image of the function $\phi(\epsilon|\omega)$,

$$\phi(\tau|\omega) = \int_{-\infty}^{\infty} \frac{d\epsilon}{2\pi} \phi(\epsilon|\omega) \exp(i\epsilon\tau). \quad (6)$$

Then, the equation (4a) takes the form

$$\left(-i\frac{d}{d\tau} - \omega \right) \phi(\tau|\omega) + \frac{1}{2}I\delta(\tau) \left(\vec{\sigma} \cdot \vec{S} \right) A = 0. \quad (7)$$

Its solution is easily found to be

$$\phi(\tau|\omega) = e^{i\omega\tau} \begin{cases} \chi, & \tau < 0 \\ \mathbf{R}(\omega)\chi, & \tau > 0 \end{cases} \quad (8)$$

with the electron-impurity scattering matrix

$$\mathbf{R}(\omega) = u(\omega) + 2v(\omega) \left(\vec{\sigma} \cdot \vec{S} \right), \quad (9a)$$

where the parameters $u(\omega)$ and $v(\omega)$ are determined by the equations

$$u + v = 1 - i \frac{\frac{1}{4}I\rho(\omega)}{1 + \frac{1}{4}I\Sigma(\omega)} \quad (9b)$$

$$u - 3v = 1 + i \frac{\frac{3}{4}I\rho(\omega)}{1 - \frac{3}{4}I\Sigma(\omega)}. \quad (9c)$$

In a metal, where an electron-impurity scattering is energy independent, one may introduce the permutation operator of electron spins, $\mathbf{P} = \delta_{\sigma_1, \sigma'_2} \delta_{\sigma_2, \sigma'_1}$ as an electron-electron scattering matrix to factorize multiparticle scattering and

to construct thus Bethe ansatz eigenfunctions of the system. In an unconventional host, multiparticle scattering is not factorized by the permutation operator because of an energy dependence of electron-impurity scattering amplitudes.

Let us introduce a two-particle scattering matrix of electrons with the energies ω_1 and ω_2 ,

$$\phi(\tau_1 > \tau_2 | \omega_1, \omega_2) = \mathbf{r}_{12}(\omega_1, \omega_2) \phi(\tau_1 < \tau_2 | \omega_1, \omega_2), \quad (10a)$$

by the most general $SU(2)$ -symmetric expression

$$\mathbf{r}(\omega_1, \omega_2) = \frac{h(\omega_1) - h(\omega_2) - i\mathbf{P}}{h(\omega_1) - h(\omega_2) - i}. \quad (10b)$$

Then multiparticle scattering in the system of host electrons is well known to be factorized at an arbitrary function $h(\omega)$, since the matrix \mathbf{r}_{ij} , where the particle index $j = 1, 2, 3$ is assumed to incorporate also its energy, obeys the Yang-Baxter factorization conditions [1,2]

$$\mathbf{r}_{12}\mathbf{r}_{13}\mathbf{r}_{23} = \mathbf{r}_{23}\mathbf{r}_{13}\mathbf{r}_{12}. \quad (11a)$$

Introducing an impurity fixes an expression for the function $h(\omega)$. To factorize multiparticle scattering in the presence of the impurity with \mathbf{R} matrix derived in Eq. (10), one needs to solve the Yang-Baxter equations involving two electrons and the impurity,

$$\mathbf{r}_{12}\mathbf{R}_{10}\mathbf{R}_{20} = \mathbf{R}_{20}\mathbf{R}_{10}\mathbf{r}_{12}, \quad (11b)$$

that gives

$$h(\omega) = \frac{u(\omega)}{v(\omega)}. \quad (11c)$$

Thus, the multiparticle scattering in the unconventional Kondo model is proven to be factorized in the auxiliary τ -space related to the particle energy, and the N -particle eigenfunctions of the model, $\Phi(\tau_1, \dots, \tau_N)$ are written in the standard BA form. The N -particle eigenfunctions in the auxiliary x -space related to the particle momentum, $\Psi(x_1, \dots, x_N)$, are found as a result of a “dressing” procedure

$$\Psi(x_1, \dots, x_N) = \int_{-\infty}^{\infty} \Phi(\tau_1, \dots, \tau_N) \prod_{j=1}^N u(x_j | \tau_j) d\tau_j, \quad (12a)$$

with the dressing function

$$u(x | \tau) = \int_C \frac{d\epsilon}{2\pi} \rho(\epsilon) e^{i[k(\epsilon)x - \epsilon\tau]}, \quad (12b)$$

where $k(\epsilon)$ is the inverse dispersion. In a metal host, where $\epsilon(k) = k$, the dressing function is nothing but the Dirac delta function, $u(x | \tau) = \delta(x - \tau)$, and hence the x and τ representations coincide.

Imposing periodic boundary conditions on the wave function $\Psi(x_1, \dots, x_N)$ on the interval of size L leads in the standard manner [1,2] to the BA equations

$$\exp(ik_j L) \varphi_c(\omega_j) = \prod_{\alpha=1}^M \frac{h_j - \lambda_\alpha - \frac{i}{2}}{h_j - \lambda_\alpha + \frac{i}{2}} \quad (13a)$$

$$\varphi_s(\lambda_\alpha) \prod_{j=1}^N \frac{\lambda_\alpha - h_j - \frac{i}{2}}{\lambda_\alpha - h_j + \frac{i}{2}} = - \prod_{\beta=1}^M \frac{\lambda_\alpha - \lambda_\beta - i}{\lambda_\alpha - \lambda_\beta + i} \quad (13b)$$

where M is the number of particles with spin “down”, $k_j \equiv k(\omega_j)$, and $h_j \equiv h(\omega_j)$. The eigenenergy E and the z component of the total spin of the system S^z are found to be

$$E = \sum_{j=1}^N \omega_j, \quad S^z = \frac{1}{2} + \frac{N}{2} - M. \quad (13c)$$

In Eqs. (13) the phase factors

$$\varphi_c(\omega) = \frac{1 + \frac{1}{4}I\Sigma'(\omega) - \frac{i}{2}\frac{1}{4}I\rho(\omega)}{1 + \frac{1}{4}I\Sigma'(\omega) + \frac{i}{2}\frac{1}{4}I\rho(\omega)} \quad (14a)$$

$$\varphi_s(\lambda) = \frac{\lambda - \frac{i}{2}}{\lambda + \frac{i}{2}} \quad (14b)$$

describe the scattering of charge and spin excitation of the host on the impurity. The equations (13) solve exactly the problem of diagonalization of the s-d exchange (Kondo) model in an unconventional host.

It should be emphasized that these equations are incomplete yet in the case of a gapped host, since they do not account for electron-impurity bound states with eigenenergies lying inside the gap. However, for a further analysis of the problem one needs to specify physical characteristic of a host, therefore we are going to address the thermodynamic properties of a Kondo impurity in unconventional Fermi systems in separated publications.

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